Formation of Intermediate Coupling Optical Polarons and Bipolarons in Two-Dimensional Systems

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Abstract. The formation of the optical polaron and bipolaron in two-dimensional (2D) systems are studied in the intermediate electron-phonon coupling regime. The total energies of 2D polaron and bipolaron are calculated by using the Buimistrov-Pekar method of canonical transformations and analyzed in the weak, intermediate and strong coupling regimes. It is shown that the electron-phonon correlation significantly reduces the total energy of 2D polaron in comparison with the energy of the strong-coupling (adiabatic) polaron. A charge carrier in polar crystals remains localized in a 2D potential well when the electron-phonon coupling constant α is greater than the critical value $\alpha_c \simeq 2.94$, which is much lower than a critical value of the electron-phonon coupling constant α for a 3D system. The critical values of the electron-phonon coupling constant α and the parameter of Coulomb repulsion between two carriers $\beta = 1/(1 - \varepsilon_\infty/\varepsilon_0)$ (where ε_∞ and ε_0 are the high frequency and static dielectric constants, respectively), which determine the bipolaron stability region, are numerically calculated. The obtained results are compared with the ones obtained by using the Feynman path integral method and the modified Lee-Low-Pines unitary transformation method.

PACS numbers: 61.50.-f, 71. 27.+a, 71.38.+i, 74.10.+v, 74.72.-h

Keywords: ionic crystals, two-dimensional systems, three electron-phonon coupling regimes, optical polarons and bipolarons Buimistrov-Pekar method, electron-phonon correlation, intermediate coupling optical polarons and bipolarons

1. Introduction

As is well known, charge carriers (electrons and holes) is ionic crystals interact with polar optical phonons and they are self-trapped at their sufficiently strong coupling to the phonons with the formation of optical polarons (called as the Pekar or Fröhlich polarons) [1, 2, 3]. One distinguishes three distinct regimes of electron-phonon coupling [2]: (i) the weak-coupling regime describes the correlated motions of the lattice atoms and the quasi-free charge carriers which remain in their initial extended state, (ii) the intermediate-coupling regime characterizes the self-trapping of a charge carrier which is bound within a potential well produced by the polarization of the lattice in the presence of the carrier and follows the atomic motions, and (iii) the strong-coupling regime describes the other condition of self-trapping under which the lattice atoms no longer follow the charge carrier motion and the self-trapping of carriers is usually treated within the adiabatic approximation (i.e. lattice atoms remain at their fixed positions). Under certain conditions, two charge carriers interacting with the lattice vibrations and with each other can form a bound state of two carriers in polar materials within a common self-trapping well. Since the attractive interaction of the electron-phonon coupling in these systems is strong enough to overcome the Coulomb repulsion between two carriers. The self-trapped state of the pair of charge carriers is termed a bipolaron. In the last few decades, the bipolaron problem has been a focus of attention due to its importance in semiconductor technology and in the bipolaronic mechanism of superconductivity (see Refs. [4, 5, 6, 7, 8, 9, 10, 11, 12]). After the discovery of the layered high-T_c cuprate superconductors, the study of bipolarons has attracted the revived interest because some researchers believe that the bipolaron is one of the possible candidate for explaining high-T_c superconductivity. The mechanism of high-T_c superconductivity of large bipolarons was proposed by Emin and Hillary [7]. This mechanism is based on the Bose-Einstein condensation of bipolarons as discussed by Schafroth [13]. Another mechanism of high-T_c superconductivity driven by the superfluid single particle and pair condensation of large bipolarons and polaron Cooper pairs was proposed in [14, 15]. The possibility of such a novel superconductivity depends on the existence of polaron and bipolarons in the superconducting materials. The above electron-phonon coupling regimes are characterized by the dimensionless Fröhlich coupling constant α. The possible ranges of the values of α characterizing the weak, intermediate and strong coupling regimes depend on the type of self-trapped charge carriers and the dimensionality of the system. The polaron and bipolaron ground state in the strong coupling limit (i.e. in the adiabatic approximation) have been studied by many authors for 3D and 2D systems [6, 7, 8, 9, 10, 11, 16, 17]. However, with decreasing α, it is necessary to take into account the electron-phonon correlation which reduces the energies of the polaron and bipolaron in comparison with those of the adiabatic polaron and bipolaron. Therefore, a quantitative treatment of the (bi)polaron problem in the intermediate-coupling regime was also a subject of numerous studies in the past three decades (see Refs [6, 8, 9, 10, 16, 18, 19]). The ground state energies

of the polaron and bipolaron have been calculated by using several approximations, such as the Feynman path integral method [6, 9, 10, 16, 20], the Lee-Low-Pines (LLP) unitary transformation method [16, 18] and the operator formalism [8, 18]. According to different intermediate coupling treatments, the formation of the polaron and bipolaron becomes possible only if the values of α are greater than the certain critical values α_c. The previous calculations have shown that the (bi)polaron is created more easily in 2D systems than in 3D ones and the stability region for bipolaron formation is much broader in 2D case as compared with 3D case. So far, calculations of the ground-state energies of the (bi)polaron, the values of α_c and the stability region of the bipolaron are not conclusive. Some of the estimated values of α_c differ greatly in magnitude. Further, the calculation methods used to study the (bi)polaron problem suffer from the certain drawbacks (see Refs. [9, 18]). In particular, the Feynman path integral method is more accurate for the calculation of the polaron energy [9, 16, 18], but it fails to describe correctly the bipolaron formation. Moreover, the functional for the bipolaron energy has rather a cumbersome form which requires the tedious numerical calculations. Therefore, it is expedient to use the another method for the calculation of the polaron and bipolaron energies in the intermediate-coupling regime. One of such methods is the Buimistrov-Pekar method [21]. In this approach, the electron-phonon correlation is taken into account through the displacement amplitude $F_{\vec{q}}(\vec{r})$ of the form:

$$F_{\vec{q}}(\vec{r}) = f_{\vec{q}} + g_{\vec{q}} \exp(-i\vec{q}\vec{r}), \tag{1}$$

where $f_{\vec{q}}$ and $g_{\vec{q}}$ are the variational parameters, which are determined from the condition for minima of the total energy, $\vec{r}$ is the electron coordinate, $\vec{q}$ is the phonon wave vector.

The second term in Eq. (1) takes into account the electron-phonon correlation effect that leads to the reduction of the energy of a 3D adiabatic polaron when $\alpha > \alpha_c$. At $\alpha < \alpha_c$ the present method leads to the delocalized state of a polaron, and the total energy of the polaron is given by $E_p = \alpha\hbar\omega_o$ (where ω_o is the longitudinal optical (LO) phonon frequency). In the Feynman path integral variational approach [20], the delocalization of the polaron at a finite value of α does not occur and the lowest polaron energy is obtained. However, at $\alpha > \alpha_c$ the Buimistrov-Pekar method taking into account an important part of the electron-phonon correlation gives also reasonable results for the energy of the polaron. The main advantage with this method is that it is simple and does not require tedious numerical calculations. Recently, the Buimistrov-Pekar method was applied to study both the free bipolaron and the bound bipolaron in 3D systems [22, 23, 24]. The existence of polarons and bipolarons in high-T_c cuprates and other materials has been indicated by several experiments [25, 26, 27, 28, 29]. The CuO_2-based layered high-T_c materials are believed to be quasi-two-dimensional systems and in an intermediate electron-phonon coupling regime. So far, the problems of the 2D polaron and bipolaron are not studied sufficiently and the possibility of formation of intermediate-coupling polarons and bipolarons in 2D systems within the Buimistrov-Pekar formalism is not explored. The aim of the present paper is to study the formation of the intermediate coupling optical polaron and bipolaron in 2D systems by using

the Buimistrov-Pekar method and to expose the important features of this method. We calculate the ground-state energies of the intermediate coupling 2D (bi)polarons, the critical values of α, the parameter of the Coulomb repulsion between two carriers $\beta = 1/(1 - \varepsilon_\infty/\varepsilon_0)$ (where ε_∞ and ε_0 are the high frequency and static dielectric constants) for the formation of 2D polaron and bipolaron. We discuss the obtained results and compare them with previous ones obtained by using the Feynman path integral method and the modified LLP unitary transformation method [16, 30].

2. Formation of intermediate-coupling polarons

The Hamiltonian and variational wave function describing the interacting system of electron (or hole) and LO phonons can be written as [22, 24]

$$H_p = -\frac{\hbar^2}{2m^*}\Delta + \sum_q \left[V_q b_q \exp(iqr) + V_q^* b_q^+ \exp(-iqr)\right] + \sum_q \hbar\omega_o b_q^+ b_q, \quad (2)$$

and

$$\Psi = \Phi_{ph}\varphi(r) = U|0\rangle\varphi(r), \quad (3)$$

where

$$U = \exp\left[\sum_q \left(F_q(r) b_q^+ - F_q^*(r) b_q\right)\right], \quad U^*U = 1, \quad \langle 0|0\rangle = 1, \quad (4)$$

$$\frac{|V_q|^2}{\hbar\omega_o} = \frac{2\pi\hbar\omega_o l_o}{L^2 q}\alpha, \quad l_o = \sqrt{\frac{\hbar}{2m^*\omega_o}}, \quad \alpha = \frac{e^2}{2\pi\omega_o l_o}\left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0}\right), \quad (5)$$

m^* is the effective mass of the carrier before polaron formation, $V_{\vec{q}}$ is the 2D form factor of the electron-phonon interaction, L^2 is the size (or surface) of the 2D system, $b_q^+(b_q)$ is the creation (annihilation) operator of the LO phonon with the wave vector $\vec{q}$ and the frequency ω_o, $\varphi(r)$ is the one-electron wave function Φ_{ph} represents the phonon part of the wave function, $|0\rangle$ is the unperturbed zero-phonon state satisfying $b_{\vec{q}}|0\rangle = 0$ and $\langle 0|0\rangle = 1$. Averaging the Hamiltonian (2) over Φ_{ph}, we have

$$\tilde{H}_p = -\frac{\hbar^2}{2m^*}\Delta + \sum_q \left[\frac{\hbar^2}{2m^*}\left|\nabla F_q(r)\right|^2 + \hbar\omega_o\left|F_q(r)\right|^2 + V_q F_q(r)\exp(iqr) + V_q^* F_q^*(r)\exp(-iqr)\right] \quad (6)$$

After substituting Eq.(1) into Eq.(6), averaging the Himiltonian (6) over $\varphi(r)$, and minimizing the energy $E_p = \langle\varphi|\tilde{H}_p|\varphi\rangle$ with respect to $f_{\vec{q}}$ and $g_{\vec{q}}$, we obtain the following functional for the total energy of a 2D polaron

$$E_p = K - \sum_q \frac{|V_q|^2}{\hbar\omega_o} W_q^2 - \sum_q \frac{|V_q|^2}{\hbar\omega_o}\frac{[1 - W_q^2]^2}{1 - W_q^2 + l_o^2 q^2}, \quad (7)$$

where

$$K = \frac{\hbar^2}{2m^*}\int d^2r \left(\frac{\partial\varphi}{\partial r}\right)^2,$$

$$W_q = \int d^2r \exp(iqr)\varphi^2(r), \sum_{\vec{q}} ... = \left(\frac{L}{2\pi}\right)^2 \int d^2q ...$$

The latter sum in Eq. (7) is the correction term arising from the electron-phonon correlation caused by the second term in Eq.(1). The functional (7) without this term ($g_{\vec{q}} = 0$) determines the energy of the strong-coupling adiabatic polaron. For simplifying the calculations, we choose the electron wave function in the form

$$\varphi(r) = N \exp(-\delta^2 r^2), \quad \pi N^2 = 2\delta^2, \quad W_q^2 = \exp(-q^2/4\delta^2) \tag{8}$$

Then we obtain the following expression for the energy (in units of $\hbar\omega_o$) of the intermediate coupling 2D polaron:

$$E_p = 2\mu^2 - \sqrt{\pi}\mu\alpha - 2\mu\alpha \int_0^\infty dt \frac{[1-\exp(-t^2)]^2}{1-\exp(-t^2)+4\mu^2 t^2}, \tag{9}$$

where $\mu = l_o\delta$.

In the weak and strong coupling limits, we obtain from Eq. (9)

$$E_p = \begin{cases} -\frac{\pi}{2}\alpha & \text{for} \quad \alpha < \alpha_c = 2.94 \\ -\frac{\pi}{8}\alpha^2 & \text{for} \quad \alpha \to \infty \end{cases} \tag{10}$$

The Feynman path integral method and the LLP unitary transformation method applied to the polaron problem, give the following expressions for the energies of the polarons [16]:

$$E_p^F = \frac{(v-w)^2}{2v} - \frac{\alpha}{2}\sqrt{\frac{\pi}{2}} \int_0^\infty dt \frac{\exp(-t)}{\sqrt{D(t)}},$$
$$D(t) = \frac{w^2}{2v^2}t + \frac{v^2-w^2}{2v^3}[1-\exp(-vt)] \tag{11}$$

and

$$E_p^{LLP} = \frac{\lambda}{2} - \alpha \int_0^\infty dt \frac{\exp[-(1-\gamma)^2 t^2/\lambda]}{1+\gamma^2 t^2}, \tag{12}$$

where v, w and λ, γ are the respective variational parameters.

The energies of the 2D polarons in the weak and strong coupling limits follow directly from Eqs. (11) and (12):

$$E_p^F = \begin{cases} -\frac{\pi}{2}\alpha - \frac{\pi^2}{216}\alpha^2 & \text{for} \quad \alpha \to 0 \\ -\frac{\pi}{8}\alpha^2 & \text{for} \quad \alpha \to \infty \end{cases} \tag{13}$$

$$E_p^{LLP} = \begin{cases} -\frac{\pi}{2}\alpha & \text{for} \quad \alpha < \alpha_c = 3.62 \\ -\frac{\pi}{8}\alpha^2 & \text{for} \quad \alpha \to \infty. \end{cases} \tag{14}$$

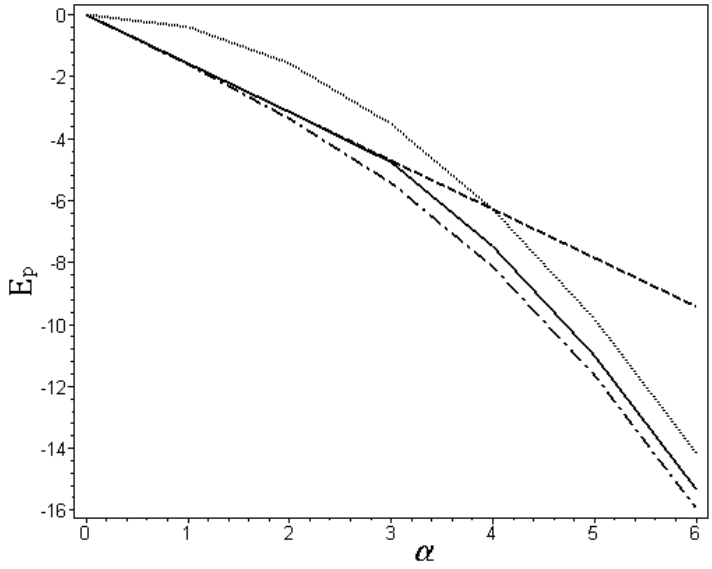

Figure 1. The energies of the 2D polarons (in units of $\hbar\omega_o$) as a function of α for the strong coupling (dotted curve) and weak coupling (dashed line) limits, calculated by using Eq. (10), for the intermediate coupling limit (solid curve), calculated by using Eq.(9). Thin solid curve calculated by the Feynman path integral method, Eq. (11).

These results can be compared with Eqs. (9) and (10). As can be seen from Eqs. (10), (13) and (14), all three methods in the strong-coupling limit give the same result. For compairing, in Fig.1, the energies of 2D polarons (in units of $\hbar\omega_o$) obtained from the Eqs. (9) and (11) are plotted as a function of α. As seen from Fig. 1, the energy of the 2D polaron calculated by taking into account the electron-phonon correlation within the Buimistrov-Pekar approximation is lower than that of the 2D adiabatic polaron. At $\alpha > \alpha_c \simeq 2.94$, a bound state of a carrier exists in 2D systems and the polaron remains localized in the 2D polarization well.

3. Formation of the intermediate-coupling bipolarons

In the bipolaron problem the total energy of the interacting system of two carriers and LO phonons is determined. The Hamiltonian and wave function describing such a system are given by

$$H_B = -\frac{\hbar^2}{2m^*}(\Delta_1 + \Delta_2) + \frac{e^2}{\varepsilon_\infty r_{12}} + \sum_q [V_q b_q(\exp(iqr_1) + \exp(iqr_2)) +$$

$$V_q^* b_q^*(\exp(-iqr_1) + \exp(-iqr_2))] + \sum_q \hbar\omega_o b_q^+ b_q \tag{15}$$

$$\Psi = \Phi_{ph}\varphi(r_1, r_2) = U|0\rangle\varphi(r_1, r_2), \tag{16}$$

where

$$U = \exp\left[\sum_q \left(F_q(r_1, r_2)b_q^+ - F_q^*(r_1, r_2)b_q\right)\right], \tag{17}$$

$\varphi(r_1, r_2)$ is the wave function of two carriers, $V_{\vec{q}}$ is the form factor of the electron-phonon interaction given by Eq. (5).

Averaging the Hamiltonian (15) over Φ_{ph}, we obtain the effective Hamiltonian

$$\tilde{H}_B = -\frac{\hbar^2}{2m^*}(\Delta_1 + \Delta_2) + \frac{e^2}{\varepsilon_\infty r_{12}} + \sum_q \left[\frac{\hbar^2}{2m^*} \left(|\nabla_1 F_q(r_1, r_2)|^2 + |\nabla_2 F_q(r_1, r_2)|^2 \right) + \hbar\omega_o |F_q(r_1, r_2)|^2 + F_q(r_1, r_2) V_q (\exp(iqr_1) + \exp(iqr_2)) + F_q^*(r_1, r_2) V_q^* (\exp(-iqr_1) + \exp(-iqr_2)) \right]. \quad (18)$$

The displacement amplitude $F_{\vec{q}}(\vec{r_1}, \vec{r_2})$ in Eq. (18), which is a generalization of that applied above to the polaron problem, can be written in the form

$$F_q(r_1, r_2) = f_q + g_q(\exp(-iqr_1) + \exp(-iqr_2)) \quad (19)$$

Substituting Eq. (19) into Eq. (18), averaging the Hamiltonian (18) over $\varphi(r_1, r_2)$, and minimizing the energy $E_B = \langle\varphi|\tilde{H}_B|\varphi\rangle$ with respect to $f_{\vec{q}}$ and $g_{\vec{q}}$, we obtain the following functional for the total energy of a 2D bipolaron

$$E_B = K_1 + K_2 + V_{12} - \sum_q \frac{|V_q|^2}{\hbar\omega_o} W_q^2 - \sum_q \frac{|V_q|^2}{\hbar\omega_o} \frac{[D_q - W_q^2]^2}{D_q - W_q^2 + 2l_0^2 q^2}, \quad (20)$$

where

$$K_{1,2} = \frac{\hbar^2}{2m^*} \int d^2r_1 d^2r_2 \left[\frac{\partial\varphi(r_1, r_2)}{\partial r_{1,2}} \right]^2, \quad V_{12} = \frac{e^2}{\varepsilon_\infty} \int \frac{\varphi^2(r_1, r_2)}{r_{12}} d^2r_1 d^2r_2,$$

$$W_q = \int d^2r_1 d^2r_2 \left[\exp(iqr_1) + \exp(iqr_2) \right] \varphi^2(r_1, r_2)$$

$$D_q = \int d^2r_1 d^2r_2 [2 + \exp(iq(r_1 - r_2)) + \exp(-iq(r_1 - r_2))] \varphi^2(r_1, r_2)$$

The constant of the Coulomb interaction $U = e^2/\varepsilon_\infty$ can be written as $U = 2\beta\sqrt{\alpha}$; where $\beta = 1/(1 - \eta)$, $\eta = \varepsilon_\infty/\varepsilon_0$. The latter sum in Eq. (20), just as in the polaron problem, is the correction term arising from the electron-phonon correlation caused by the second term in Eq. (19). The functional (20) without this term ($g_{\vec{q}} = 0$) determines the energy of the strong-coupling adiabatic bipolaron. For calculation of the bipolaron energy in the strong-coupling limit, we choose the following two trial wave functions:

$$\varphi(r_1, r_2) = N \exp(-\delta^2(r_1^2 + r_2^2))[1 + \gamma\delta^2 r_{12}^2], \quad \gamma > 0 \quad (21)$$

$$\varphi(r_1, r_2) = N \exp(-\delta^2(r_1^2 + r_2^2))[1 - b\exp(-\gamma\delta^2 r_{12}^2)], \quad \gamma > 0, \quad b < 1 \quad (22)$$

The bipolaron is stabile when the bipolaron energy is lower than twice the polaron energy, i.e., the bipolaron stability regions is determined by the inequality $E_B < 2E_p$. At $\alpha \to \infty$, the bipolaron energy calculated with the use of the trial wave function (21) is approximately 2.5 times larger than the polaron energy $E_p = -(\pi/8)\alpha^2$, i.e. $E_B/2E_p \approx 1.25$. While the value of E_p calculated in the strong-coupling limit ($\alpha \to \infty$) with the use of the trial wave function (22) is equal to $E_B \simeq 2.58E_p$, so that $E_B/2E_p \simeq 1.29$. In the intermediate coupling regime, the energy of the 2D bipolaron is

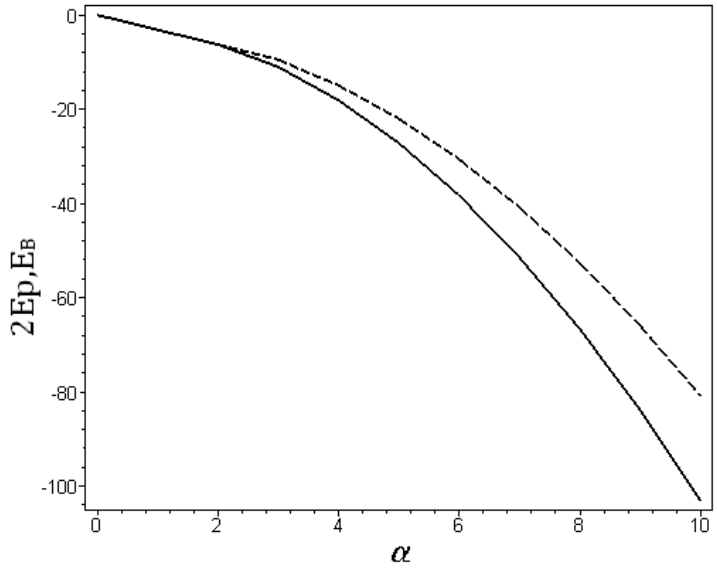

Figure 2. The 2D bipolaron energy (solid curve), calculated with using the Eq. (20), and the double 2D polaron energy (dashed curve), calculated with using the Eq. (9), as a function of α and in units of $\hbar\omega_o$.

calculated by using the trial wave function (22). The results for the limit case $\beta = 1$ ($\eta = 0$) are shown in Fig.2. In this approximation the 2D bipolaron is stable for $\alpha > \alpha_c = 2.94$ which is comparable with the 2D results obtained by using the Feynman path integral method [9]. With increasing α, the bipolaron stability region is enlarged. For example, at $\alpha = 5$ and 10 the values of the parameter β corresponding to the bipolaron formation region lie in the intervals $1 < \beta < 1.201$ and $1 < \beta < 1.209$, respectively. For the cases $\alpha = 5$ and 10 the 2D bipolarons are stable at $\eta < \eta_c = 0.167$ and $\eta < \eta_c = 0.173$, respectively.

4. Conclusions

In this work we have studied the formation of intermediate-coupling optical polarons and bipolarons in 2D systems. The total energies of the 2D polaron and bipolaron are calculated by using the Buimistrov-Pekar method of canonical transformations. It is shown that this method allows us to take into account the effects of the electron-phonon correlation on the energies of the 2D (bi)polaron for any values of the electron-phonon coupling constant α and to derive the new expression for the polaron energy and limits for strong and weak coupling. In the strong-coupling limit the Buimistrov-Pekar method, the Feynman path integral method and the LLP unitary transformation method give the same result for the polaron energy. Our numerical results show that below a critical value α_c, the charge carriers are quasi-free (i.e. delocalized) electrons or holes, and only at $\alpha > \alpha_c \simeq 2.94$ (bi)polarons exist in 2D polar materials. The above critical values α_c and η_c are also close to the ones obtained by using the Feynman path integral method.

Note that for calculation of the energies of 2D polaron and bipolaron were used simple trial wave functions. Therefore, the values of the (bi)polaron energies, α_c and η_c obtained by these wave functions are approximate ones. For obtaining more precise values of these parameters, it is necessary to use more flexible wave functions, such as, for example, a sum of Gussians [24].

Acknowledgments

We would like to thank B. Yavidov for his careful reading of the manuscript. We are grateful to O.K. Ganiev for his technical assistance. This work is supported by the Foundation of the Fundamental Research of Uzbek Academy of Sciences grant FA-F2-F070.

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Abstract. The formation of the optical polaron and bipolaron in two-dimensional (2D) systems are studied in the intermediate electron-phonon coupling regime. The total energies of 2D polaron and bipolaron are calculated by using the Buimistrov-Pekar method of canonical transformations and analyzed in the weak, intermediate and strong coupling regimes. It is shown that the electron-phonon correlation significantly reduces the total energy of 2D polaron in comparison with the energy of the strong-coupling (adiabatic) polaron. A charge carrier in polar crystals remains localized in a 2D potential well when the electron-phonon coupling constant α is greater than the critical value $\alpha_c \simeq 2.94$, which is much lower than a critical value of the electron-phonon coupling constant α for a 3D system. The critical values of the electron-phonon coupling constant α and the parameter of Coulomb repulsion between two carriers $\beta = 1/(1 - \varepsilon_\infty/\varepsilon_0)$ (where ε_∞ and ε_0 are the high frequency and static dielectric constants, respectively), which determine the bipolaron stability region, are numerically calculated. The obtained results are compared with the ones obtained by using the Feynman path integral method and the modified Lee-Low-Pines unitary transformation method.

PACS numbers: 61.50.-f, 71. 27.+a, 71.38.+i, 74.10.+v, 74.72.-h

Keywords: ionic crystals, two-dimensional systems, three electron-phonon coupling regimes, optical polarons and bipolarons Buimistrov-Pekar method, electron-phonon correlation, intermediate coupling optical polarons and bipolarons

1. Introduction

As is well known, charge carriers (electrons and holes) is ionic crystals interact with polar optical phonons and they are self-trapped at their sufficiently strong coupling to the phonons with the formation of optical polarons (called as the Pekar or Fröhlich polarons) [1, 2, 3]. One distinguishes three distinct regimes of electron-phonon coupling [2]: (i) the weak-coupling regime describes the correlated motions of the lattice atoms and the quasi-free charge carriers which remain in their initial extended state, (ii) the intermediate-coupling regime characterizes the self-trapping of a charge carrier which is bound within a potential well produced by the polarization of the lattice in the presence of the carrier and follows the atomic motions, and (iii) the strong-coupling regime describes the other condition of self-trapping under which the lattice atoms no longer follow the charge carrier motion and the self-trapping of carriers is usually treated within the adiabatic approximation (i.e. lattice atoms remain at their fixed positions). Under certain conditions, two charge carriers interacting with the lattice vibrations and with each other can form a bound state of two carriers in polar materials within a common self-trapping well. Since the attractive interaction of the electron-phonon coupling in these systems is strong enough to overcome the Coulomb repulsion between two carriers. The self-trapped state of the pair of charge carriers is termed a bipolaron. In the last few decades, the bipolaron problem has been a focus of attention due to its importance in semiconductor technology and in the bipolaronic mechanism of superconductivity (see Refs. [4, 5, 6, 7, 8, 9, 10, 11, 12]). After the discovery of the layered high-T_c cuprate superconductors, the study of bipolarons has attracted the revived interest because some researchers believe that the bipolaron is one of the possible candidate for explaining high-T_c superconductivity. The mechanism of high-T_c superconductivity of large bipolarons was proposed by Emin and Hillary [7]. This mechanism is based on the Bose-Einstein condensation of bipolarons as discussed by Schafroth [13]. Another mechanism of high-T_c superconductivity driven by the superfluid single particle and pair condensation of large bipolarons and polaron Cooper pairs was proposed in [14, 15]. The possibility of such a novel superconductivity depends on the existence of polaron and bipolarons in the superconducting materials. The above electron-phonon coupling regimes are characterized by the dimensionless Fröhlich coupling constant α. The possible ranges of the values of α characterizing the weak, intermediate and strong coupling regimes depend on the type of self-trapped charge carriers and the dimensionality of the system. The polaron and bipolaron ground state in the strong coupling limit (i.e. in the adiabatic approximation) have been studied by many authors for 3D and 2D systems [6, 7, 8, 9, 10, 11, 16, 17]. However, with decreasing α, it is necessary to take into account the electron-phonon correlation which reduces the energies of the polaron and bipolaron in comparison with those of the adiabatic polaron and bipolaron. Therefore, a quantitative treatment of the (bi)polaron problem in the intermediate-coupling regime was also a subject of numerous studies in the past three decades (see Refs [6, 8, 9, 10, 16, 18, 19]). The ground state energies

of the polaron and bipolaron have been calculated by using several approximations, such as the Feynman path integral method [6, 9, 10, 16, 20], the Lee-Low-Pines (LLP) unitary transformation method [16, 18] and the operator formalism [8, 18]. According to different intermediate coupling treatments, the formation of the polaron and bipolaron becomes possible only if the values of α are greater than the certain critical values α_c. The previous calculations have shown that the (bi)polaron is created more easily in 2D systems than in 3D ones and the stability region for bipolaron formation is much broader in 2D case as compared with 3D case. So far, calculations of the ground-state energies of the (bi)polaron, the values of α_c and the stability region of the bipolaron are not conclusive. Some of the estimated values of α_c differ greatly in magnitude. Further, the calculation methods used to study the (bi)polaron problem suffer from the certain drawbacks (see Refs. [9, 18]). In particular, the Feynman path integral method is more accurate for the calculation of the polaron energy [9, 16, 18], but it fails to describe correctly the bipolaron formation. Moreover, the functional for the bipolaron energy has rather a cumbersome form which requires the tedious numerical calculations. Therefore, it is expedient to use the another method for the calculation of the polaron and bipolaron energies in the intermediate-coupling regime. One of such methods is the Buimistrov-Pekar method [21]. In this approach, the electron-phonon correlation is taken into account through the displacement amplitude $F_{\vec{q}}(\vec{r})$ of the form:

$$F_{\vec{q}}(\vec{r}) = f_{\vec{q}} + g_{\vec{q}} \exp(-i\vec{q}\vec{r}), \tag{1}$$

where $f_{\vec{q}}$ and $g_{\vec{q}}$ are the variational parameters, which are determined from the condition for minima of the total energy, $\vec{r}$ is the electron coordinate, $\vec{q}$ is the phonon wave vector.

The second term in Eq. (1) takes into account the electron-phonon correlation effect that leads to the reduction of the energy of a 3D adiabatic polaron when $\alpha > \alpha_c$. At $\alpha < \alpha_c$ the present method leads to the delocalized state of a polaron, and the total energy of the polaron is given by $E_p = \alpha\hbar\omega_o$ (where ω_o is the longitudinal optical (LO) phonon frequency). In the Feynman path integral variational approach [20], the delocalization of the polaron at a finite value of α does not occur and the lowest polaron energy is obtained. However, at $\alpha > \alpha_c$ the Buimistrov-Pekar method taking into account an important part of the electron-phonon correlation gives also reasonable results for the energy of the polaron. The main advantage with this method is that it is simple and does not require tedious numerical calculations. Recently, the Buimistrov-Pekar method was applied to study both the free bipolaron and the bound bipolaron in 3D systems [22, 23, 24]. The existence of polarons and bipolarons in high-T_c cuprates and other materials has been indicated by several experiments [25, 26, 27, 28, 29]. The CuO_2-based layered high-T_c materials are believed to be quasi-two-dimensional systems and in an intermediate electron-phonon coupling regime. So far, the problems of the 2D polaron and bipolaron are not studied sufficiently and the possibility of formation of intermediate-coupling polarons and bipolarons in 2D systems within the Buimistrov-Pekar formalism is not explored. The aim of the present paper is to study the formation of the intermediate coupling optical polaron and bipolaron in 2D systems by using

the Buimistrov-Pekar method and to expose the important features of this method. We calculate the ground-state energies of the intermediate coupling 2D (bi)polarons, the critical values of α, the parameter of the Coulomb repulsion between two carriers $\beta = 1/(1 - \varepsilon_\infty/\varepsilon_0)$ (where ε_∞ and ε_0 are the high frequency and static dielectric constants) for the formation of 2D polaron and bipolaron. We discuss the obtained results and compare them with previous ones obtained by using the Feynman path integral method and the modified LLP unitary transformation method [16, 30].

2. Formation of intermediate-coupling polarons

The Hamiltonian and variational wave function describing the interacting system of electron (or hole) and LO phonons can be written as [22, 24]

$$H_p = -\frac{\hbar^2}{2m^*}\Delta + \sum_q \left[V_q b_q \exp(iqr) + V_q^* b_q^+ \exp(-iqr)\right] + \sum_q \hbar\omega_o b_q^+ b_q, \quad (2)$$

and

$$\Psi = \Phi_{ph}\varphi(r) = U|0\rangle\varphi(r), \quad (3)$$

where

$$U = \exp\left[\sum_q \left(F_q(r) b_q^+ - F_q^*(r) b_q\right)\right], \quad U^*U = 1, \quad \langle 0|0\rangle = 1, \quad (4)$$

$$\frac{|V_q|^2}{\hbar\omega_o} = \frac{2\pi\hbar\omega_o l_o}{L^2 q}\alpha, \quad l_o = \sqrt{\frac{\hbar}{2m^*\omega_o}}, \quad \alpha = \frac{e^2}{2\pi\omega_o l_o}\left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0}\right), \quad (5)$$

m^* is the effective mass of the carrier before polaron formation, $V_{\vec{q}}$ is the 2D form factor of the electron-phonon interaction, L^2 is the size (or surface) of the 2D system, $b_q^+(b_q)$ is the creation (annihilation) operator of the LO phonon with the wave vector $\vec{q}$ and the frequency ω_o, $\varphi(r)$ is the one-electron wave function Φ_{ph} represents the phonon part of the wave function, $|0\rangle$ is the unperturbed zero-phonon state satisfying $b_{\vec{q}}|0\rangle = 0$ and $\langle 0|0\rangle = 1$. Averaging the Hamiltonian (2) over Φ_{ph}, we have

$$\tilde{H}_p = -\frac{\hbar^2}{2m^*}\Delta + \sum_q \left[\frac{\hbar^2}{2m^*}\left|\nabla F_q(r)\right|^2 + \hbar\omega_o\left|F_q(r)\right|^2 + V_q F_q(r)\exp(iqr) + V_q^* F_q^*(r)\exp(-iqr)\right] \quad (6)$$

After substituting Eq.(1) into Eq.(6), averaging the Himiltonian (6) over $\varphi(r)$, and minimizing the energy $E_p = \langle\varphi|\tilde{H}_p|\varphi\rangle$ with respect to $f_{\vec{q}}$ and $g_{\vec{q}}$, we obtain the following functional for the total energy of a 2D polaron

$$E_p = K - \sum_q \frac{|V_q|^2}{\hbar\omega_o} W_q^2 - \sum_q \frac{|V_q|^2}{\hbar\omega_o}\frac{[1 - W_q^2]^2}{1 - W_q^2 + l_o^2 q^2}, \quad (7)$$

where

$$K = \frac{\hbar^2}{2m^*}\int d^2r \left(\frac{\partial\varphi}{\partial r}\right)^2,$$

$$W_q = \int d^2r \exp(iqr)\varphi^2(r), \sum_{\vec{q}} ... = \left(\frac{L}{2\pi}\right)^2 \int d^2q ...$$

The latter sum in Eq. (7) is the correction term arising from the electron-phonon correlation caused by the second term in Eq.(1). The functional (7) without this term ($g_{\vec{q}} = 0$) determines the energy of the strong-coupling adiabatic polaron. For simplifying the calculations, we choose the electron wave function in the form

$$\varphi(r) = N \exp(-\delta^2 r^2), \quad \pi N^2 = 2\delta^2, \quad W_q^2 = \exp(-q^2/4\delta^2) \tag{8}$$

Then we obtain the following expression for the energy (in units of $\hbar\omega_o$) of the intermediate coupling 2D polaron:

$$E_p = 2\mu^2 - \sqrt{\pi}\mu\alpha - 2\mu\alpha \int_0^\infty dt \frac{[1-\exp(-t^2)]^2}{1-\exp(-t^2)+4\mu^2 t^2}, \tag{9}$$

where $\mu = l_o\delta$.

In the weak and strong coupling limits, we obtain from Eq. (9)

$$E_p = \begin{cases} -\frac{\pi}{2}\alpha & \text{for} \quad \alpha < \alpha_c = 2.94 \\ -\frac{\pi}{8}\alpha^2 & \text{for} \quad \alpha \to \infty \end{cases} \tag{10}$$

The Feynman path integral method and the LLP unitary transformation method applied to the polaron problem, give the following expressions for the energies of the polarons [16]:

$$E_p^F = \frac{(v-w)^2}{2v} - \frac{\alpha}{2}\sqrt{\frac{\pi}{2}} \int_0^\infty dt \frac{\exp(-t)}{\sqrt{D(t)}},$$
$$D(t) = \frac{w^2}{2v^2}t + \frac{v^2-w^2}{2v^3}[1-\exp(-vt)] \tag{11}$$

and

$$E_p^{LLP} = \frac{\lambda}{2} - \alpha \int_0^\infty dt \frac{\exp[-(1-\gamma)^2 t^2/\lambda]}{1+\gamma^2 t^2}, \tag{12}$$

where v, w and λ, γ are the respective variational parameters.

The energies of the 2D polarons in the weak and strong coupling limits follow directly from Eqs. (11) and (12):

$$E_p^F = \begin{cases} -\frac{\pi}{2}\alpha - \frac{\pi^2}{216}\alpha^2 & \text{for} \quad \alpha \to 0 \\ -\frac{\pi}{8}\alpha^2 & \text{for} \quad \alpha \to \infty \end{cases} \tag{13}$$

$$E_p^{LLP} = \begin{cases} -\frac{\pi}{2}\alpha & \text{for} \quad \alpha < \alpha_c = 3.62 \\ -\frac{\pi}{8}\alpha^2 & \text{for} \quad \alpha \to \infty. \end{cases} \tag{14}$$

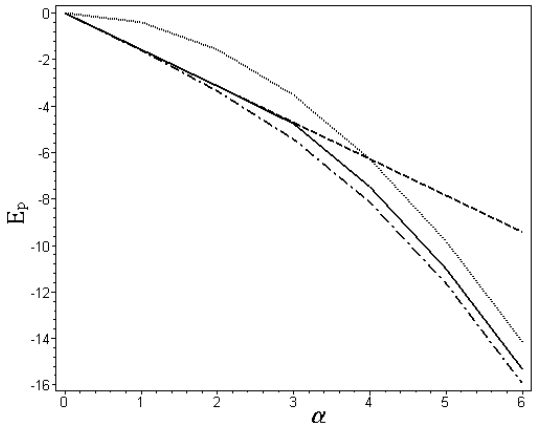

Figure 1. The energies of the 2D polarons (in units of $\hbar\omega_o$) as a function of α for the strong coupling (dotted curve) and weak coupling (dashed line) limits, calculated by using Eq. (10), for the intermediate coupling limit (solid curve), calculated by using Eq.(9). Thin solid curve calculated by the Feynman path integral method, Eq. (11).

These results can be compared with Eqs. (9) and (10). As can be seen from Eqs. (10), (13) and (14), all three methods in the strong-coupling limit give the same result. For compairing, in Fig.1, the energies of 2D polarons (in units of $\hbar\omega_o$) obtained from the Eqs. (9) and (11) are plotted as a function of α. As seen from Fig. 1, the energy of the 2D polaron calculated by taking into account the electron-phonon correlation within the Buimistrov-Pekar approximation is lower than that of the 2D adiabatic polaron. At $\alpha > \alpha_c \simeq 2.94$, a bound state of a carrier exists in 2D systems and the polaron remains localized in the 2D polarization well.

3. Formation of the intermediate-coupling bipolarons

In the bipolaron problem the total energy of the interacting system of two carriers and LO phonons is determined. The Hamiltonian and wave function describing such a system are given by

$$H_B = -\frac{\hbar^2}{2m^*}(\Delta_1 + \Delta_2) + \frac{e^2}{\varepsilon_\infty r_{12}} + \sum_q [V_q b_q(\exp(iqr_1) + \exp(iqr_2)) +$$
$$V_q^* b_q^*(\exp(-iqr_1) + \exp(-iqr_2))] + \sum_q \hbar\omega_o b_q^+ b_q \tag{15}$$

$$\Psi = \Phi_{ph}\varphi(r_1, r_2) = U|0\rangle\varphi(r_1, r_2), \tag{16}$$

where

$$U = \exp\left[\sum_q \left(F_q(r_1, r_2)b_q^+ - F_q^*(r_1, r_2)b_q\right)\right], \tag{17}$$

$\varphi(r_1, r_2)$ is the wave function of two carriers, $V_{\vec{q}}$ is the form factor of the electron-phonon interaction given by Eq. (5).

Averaging the Hamiltonian (15) over Φ_{ph}, we obtain the effective Hamiltonian

$$\tilde{H}_B = -\frac{\hbar^2}{2m^*}(\Delta_1+\Delta_2) + \frac{e^2}{\varepsilon_\infty r_{12}} + \sum_q \left[\frac{\hbar^2}{2m^*}\left(|\nabla_1 F_q(r_1,r_2)|^2 + |\nabla_2 F_q(r_1,r_2)|^2\right) + \hbar\omega_o |F_q(r_1,r_2)|^2 + F_q(r_1,r_2)V_q(\exp(iqr_1)+\exp(iqr_2)) + F_q^*(r_1,r_2)V_q^*(\exp(-iqr_1)+\exp(-iqr_2))\right]. \quad (18)$$

The displacement amplitude $F_{\vec{q}}(\vec{r}_1,\vec{r}_2)$ in Eq. (18), which is a generalization of that applied above to the polaron problem, can be written in the form

$$F_q(r_1,r_2) = f_q + g_q(\exp(-iqr_1)+\exp(-iqr_2)) \quad (19)$$

Substituting Eq. (19) into Eq. (18), averaging the Hamiltonian (18) over $\varphi(r_1,r_2)$, and minimizing the energy $E_B = \langle\varphi|\tilde{H}_B|\varphi\rangle$ with respect to $f_{\vec{q}}$ and $g_{\vec{q}}$, we obtain the following functional for the total energy of a 2D bipolaron

$$E_B = K_1 + K_2 + V_{12} - \sum_q \frac{|V_q|^2}{\hbar\omega_o} W_q^2 - \sum_q \frac{|V_q|^2}{\hbar\omega_o}\frac{[D_q - W_q^2]^2}{D_q - W_q^2 + 2l_0^2q^2}, \quad (20)$$

where

$$K_{1,2} = \frac{\hbar^2}{2m^*}\int d^2r_1 d^2r_2 \left[\frac{\partial\varphi(r_1,r_2)}{\partial r_{1,2}}\right]^2, \quad V_{12} = \frac{e^2}{\varepsilon_\infty}\int \frac{\varphi^2(r_1,r_2)}{r_{12}} d^2r_1 d^2r_2,$$

$$W_q = \int d^2r_1 d^2r_2 \left[\exp(iqr_1)+\exp(iqr_2)\right]\varphi^2(r_1,r_2)$$

$$D_q = \int d^2r_1 d^2r_2 [2+\exp(iq(r_1-r_2))+\exp(-iq(r_1-r_2))]\varphi^2(r_1,r_2)$$

The constant of the Coulomb interaction $U = e^2/\varepsilon_\infty$ can be written as $U = 2\beta\sqrt{\alpha}$; where $\beta = 1/(1-\eta)$, $\eta = \varepsilon_\infty/\varepsilon_0$. The latter sum in Eq. (20), just as in the polaron problem, is the correction term arising from the electron-phonon correlation caused by the second term in Eq. (19). The functional (20) without this term ($g_{\vec{q}} = 0$) determines the energy of the strong-coupling adiabatic bipolaron. For calculation of the bipolaron energy in the strong-coupling limit, we choose the following two trial wave functions:

$$\varphi(r_1,r_2) = N\exp(-\delta^2(r_1^2+r_2^2))[1+\gamma\delta^2 r_{12}^2], \quad \gamma > 0 \quad (21)$$

$$\varphi(r_1,r_2) = N\exp(-\delta^2(r_1^2+r_2^2))[1-b\exp(-\gamma\delta^2 r_{12}^2)], \quad \gamma > 0, \quad b < 1 \quad (22)$$

The bipolaron is stabile when the bipolaron energy is lower than twice the polaron energy, i.e., the bipolaron stability regions is determined by the inequality $E_B < 2E_p$. At $\alpha \to \infty$, the bipolaron energy calculated with the use of the trial wave function (21) is approximately 2.5 times larger than the polaron energy $E_p = -(\pi/8)\alpha^2$, i.e. $E_B/2E_p \approx 1.25$. While the value of E_p calculated in the strong-coupling limit ($\alpha \to \infty$) with the use of the trial wave function (22) is equal to $E_B \simeq 2.58E_p$, so that $E_B/2E_p \simeq 1.29$. In the intermediate coupling regime, the energy of the 2D bipolaron is calculated by using the trial wave function (22). The results for the limit case $\beta = 1$ ($\eta = 0$) are shown in Fig.2. In this approximation the 2D bipolaron is stable for

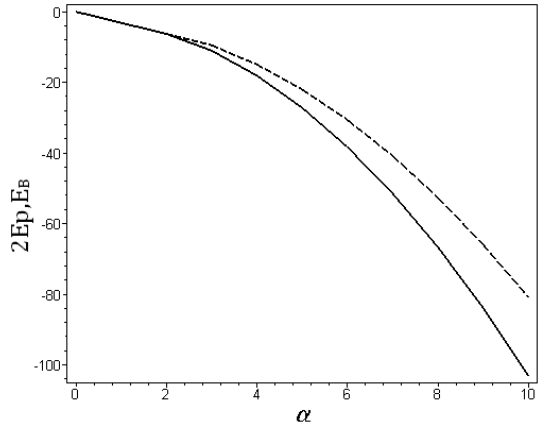

Figure 2. The 2D bipolaron energy (solid curve), calculated with using the Eq. (20), and the double 2D polaron energy (dashed curve), calculated with using the Eq. (9), as a function of α and in units of $\hbar\omega_o$.

$\alpha > \alpha_c = 2.94$ which is comparable with the 2D results obtained by using the Feynman path integral method [9]. With increasing α, the bipolaron stability region is enlarged. For example, at $\alpha = 5$ and 10 the values of the parameter β corresponding to the bipolaron formation region lie in the intervals $1 < \beta < 1.201$ and $1 < \beta < 1.209$, respectively. For the cases $\alpha = 5$ and 10 the 2D bipolarons are stable at $\eta < \eta_c = 0.167$ and $\eta < \eta_c = 0.173$, respectively.

4. Conclusions

In this work we have studied the formation of intermediate-coupling optical polarons and bipolarons in 2D systems. The total energies of the 2D polaron and bipolaron are calculated by using the Buimistrov-Pekar method of canonical transformations. It is shown that this method allows us to take into account the effects of the electron-phonon correlation on the energies of the 2D (bi)polaron for any values of the electron-phonon coupling constant α and to derive the new expression for the polaron energy and limits for strong and weak coupling. In the strong-coupling limit the Buimistrov-Pekar method, the Feynman path integral method and the LLP unitary transformation method give the same result for the polaron energy. Our numerical results show that below a critical value α_c, the charge carriers are quasi-free (i.e. delocalized) electrons or holes, and only at $\alpha > \alpha_c \simeq 2.94$ (bi)polarons exist in 2D polar materials. The above critical values α_c and η_c are also close to the ones obtained by using the Feynman path integral method.

Note that for calculation of the energies of 2D polaron and bipolaron were used simple trial wave functions. Therefore, the values of the (bi)polaron energies, α_c and η_c obtained by these wave functions are approximate ones. For obtaining more precise values of these parameters, it is necessary to use more flexible wave functions, such as, for example, a sum of Gussians [24].

Acknowledgments

We would like to thank B. Yavidov for his careful reading of the manuscript. We are grateful to O.K. Ganiev for his technical assistance. This work is supported by the Foundation of the Fundamental Research of Uzbek Academy of Sciences grant FA-F2-F070.

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